

Table 1: Wyckoff site: 4a, site symmetry: $\bar{3}$.

No.	position	mapping
1	$[x, x, x]$	[1,5,6]
2	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[2,10,11]
3	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	[3,7,12]
4	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[4,8,9]

Table 2: Wyckoff site: 12b, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[2]
3	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[4]
5	$[z, x, y]$	[5]
6	$[y, z, x]$	[6]
7	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[7]
8	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[8]
9	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[9]
10	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[10]
11	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[11]
12	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[12]